REMARKS

The applicant responds to the final office action dated April 23, 2003, and has put the case in condition for allowance in accordance with the action.

The action stated that claims 5, 9-10, and 12-14 would be allowable if rewritten in independent form.

Independent Claims

Independent claims 1-3 have been cancelled.

The action stated that claims 5, 9-10, and 12 would be allowable if rewritten in independent form. Claims 5, 9-10, and 12 have been recast in independent form. New independent <u>system</u> claim 20 and new independent <u>computer software</u> claim 21 have been added that correspond to allowable <u>method</u> claim 5.

Dependent Claims

Dependent claim 4 has been cancelled.

The action stated that claims 13-14 would be allowable if rewritten in independent form. Dependent claims 13-14 already depend from allowable claim 12, which has been recast in independent form.

Dependent claims 6-8, 11, and 15-18 have been amended to depend from allowable claim 5. New dependent claim 19 (corresponding to cancelled dependent claim 4) has been added to depend from allowable claim 5.

The applicant submits that the application is in condition for allowance, which action is requested.

The Examiner is encouraged to telephone the undersigned to discuss any matters in furtherance of the prosecution of the subject application.
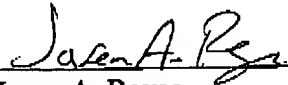
Applicant(s): Harold E. Helson   PATENT
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The Commissioner is hereby authorized to charge any fee deficiency, or credit any

overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

Dated: June 30, 2003

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Replacement Pages for Claims 1-21
(MARKED TO SHOW CHANGES)

~~1.   A method for use in deriving fixed-bond information, comprising:~~

~~analyzing a Kekulé structure representation of a chemical structure;~~

~~identifying, based on valence information, a plurality of fixed-bond representation~~ ~~candidates for at least a portion of the chemical structure;~~

~~evaluating at least a subset of the fixed bond representation candidates;~~

~~selecting from among the plurality of fixed bond representation candidates based on the~~ ~~evaluation; and~~

~~producing fixed bond information based on the selection.~~

~~2.   A system for use in deriving fixed bond information, comprising:~~

~~an analyzer analyzing a Kekulé structure representation of a chemical structure;~~

~~an identifier identifying, based on valence information, a plurality of fixed bond~~ ~~representation candidates for at least a portion of the chemical structure;~~

~~an evaluator evaluating at least a subset of the fixed bond representation candidates;~~

~~a selector electing from among the plurality of fixed bond representation candidates~~ ~~based on the evaluation; and~~

~~a producer producing fixed bond information based on the selection.~~

~~3.   Computer software, residing on a computer-readable storage medium, comprising~~ ~~a set of instructions for use in a computer system to help cause the computer system to derive~~ ~~fixed bond information, the instructions causing the system to:~~

~~analyze a Kekulé structure representation of a chemical structure;~~

~~identify, based on valence information, a plurality of fixed bond representation~~ ~~candidates for at least a portion of the chemical structure;~~

~~evaluate at least a subset of the fixed bond representation candidates; and~~

~~select from among the plurality of fixed bond representation candidates based on the~~ ~~evaluation; and~~

~~produce fixed bond information based on the selection.~~

~~4.   The method of claim 1, wherein at least a portion of the Kekulé structure~~ ~~representation describes a monocyclic ring system.~~

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5.   [The method of claim 1,] <u>A method for use in deriving fixed bond information,</u>
<u>comprising:</u>

     <u>analyzing a Kekulé structure representation of a chemical structure;</u>

     <u>identifying, based on valence information, a plurality of fixed bond representation</u>
<u>candidates for at least a portion of the chemical structure;</u>

     <u>evaluating at least a subset of the fixed bond representation candidates;</u>

     <u>selecting from among the plurality of fixed bond representation candidates based on the</u>
<u>evaluation; and</u>

     <u>producing fixed bond information based on the selection,</u>

     wherein at least a portion of the Kekulé structure representation describes a polycyclic
ring system,

6.   The method of claim [1] <u>5</u>, wherein at least a portion of the Kekulé structure
representation describes a ring system with a hetero substitution pattern.

7.   The method of claim [1] <u>5</u>, wherein at least a portion of the Kekulé structure
representation describes a non-cyclic system.

8.   The method of claim [1] <u>5</u>, wherein at least a portion of the Kekulé structure
representation describes an acyclic system.

9.   [The method of claim 1, further comprising:] <u>A method for use in deriving fixed</u>
<u>bond information, comprising:</u>

     <u>analyzing a Kekulé structure representation of a chemical structure;</u>

     <u>identifying, based on valence information, a plurality of fixed bond representation</u>
<u>candidates for at least a portion of the chemical structure;</u>

     <u>evaluating at least a subset of the fixed bond representation candidates;</u>

     <u>selecting from among the plurality of fixed bond representation candidates based on the</u>
<u>evaluation;</u>

     <u>producing fixed bond information based on the selection; and</u>

     based on the fixed bond information, producing a fixed bond representation that includes
a pair of opposite charges lacked by the Kekulé structure representation.

10.   [The method of claim 1, further comprising:] <u>A method for use in deriving fixed</u>
<u>bond information, comprising:</u>

     <u>analyzing a Kekulé structure representation of a chemical structure;</u>

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection; and

based on the fixed bond information, producing a fixed bond representation that includes a pair of radicals lacked by the Kekulé structure representation.

11.   The method of claim [1] 5, further comprising:

queuing at least a subset of the candidates by priority.

12.   [The method of claim 1, further comprising:] A method for use in deriving fixed bond information, comprising:

analyzing a Kekulé structure representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection; and

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the Kekulé structure representation.

13.   The method of claim 12, wherein the table is configured to allow additional elements and values to be added.

14.   The method of claim 12, wherein the table is configured to allow additional elements and values to be added to apply to any chemical element.

15.   The method of claim [1] 5, further comprising:

deriving electronic state and valence distributions information together with analyzing the Kekulé structure representation.

16.   The method of claim [1] 5, further comprising:

determining whether it is practical to produce a fixed bond representation of the chemical structure.

17.   The method of claim [1] 5, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18.   The method of claim [1] 5, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.

19.   The method of claim 5, wherein at least a portion of the Kekulé structure representation describes a monocyclic ring system.

20.   A system for use in deriving fixed bond information, comprising:

an analyzer analyzing a Kekulé structure representation of a chemical structure;

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates;

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer producing fixed bond information based on the selection;

wherein at least a portion of the Kekulé structure representation describes a polycyclic ring system.

21.   Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a Kekulé structure representation of a chemical structure;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; and

select from among the plurality of fixed bond representation candidates based on the evaluation; and

produce fixed bond information based on the selection;

wherein at least a portion of the Kekulé structure representation describes a polycyclic

ring system.